I built both MSVC and ICC windows builds. When GMX_ACCELERATION = SSE (the default), mdrun.exe crashes. I rebuilt with GMX_ACCELERATION = None, and things run fine. x86-64-ASM was enabled for all builds. Is GMX_ACCELERATION=SSE a problem with 64 bit builds?

I tried both PME and GBSA simulations.

Any ideas? I've attached a broken TPR (gbsa). Also, here is tail of my md.log

At this point, it's also possible I'm doing something wrong on my end, as this is the first time I've successfully compiled a windows 64 bit gromacs.

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Testing x86_64 SSE support... present.

Removing pbc first time

+++ PLEASE READ AND CITE THE FOLLOWING REFERENCE +++
J. P. Ryckaert and G. Ciccotti and H. J. C. Berendsen
Numerical Integration of the Cartesian Equations of Motion of a System with Constraints; Molecular Dynamics of n-Alkanes
J. Comp. Phys. 23 (1977) pp. 327-341
--------- -------- --- Thank You --- -------- --------

+++ PLEASE READ AND CITE THE FOLLOWING REFERENCE +++
S. Miyamoto and P. A. Kollman
SETTLE: An Analytical Version of the SHAKE and RATTLE Algorithms for Rigid Water Models
--------- -------- --- Thank You --- -------- --------

History

#1 - 08/18/2010 01:25 AM - Erik Lindahl
This was a (small) bug in the intel syntax assembly files which we only use with nasm, but with nasm it affected any x86 build (OS X too). It's fixed now in commit 97d3a2b15f69eb315c9639ac3b9f4538f3b7cf7.